WEST Search History

Hide Items | Restore | Clear | Cancel

DATE: Tuesday, April 06, 2004

Hide?	Set Name	Query	Hit Count
	DB=PGPB,USPT,EPAB,JPAB,DWPI; PLUR=YES; OP=ADJ		
☐	L8	l3 and l4	4
☐	L7	l6 and rhodamin$6.ab.	6
☐	L6	l4 and therap$6	139
☐	L5	l3 and l4L4	0
☐	L4	l2 near5 salt	485
☐	L3	photodynamic and L2	329
☐	L2	rhodamine$	25309
☐	L1	us-5556992-$.did.	2

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     (FILE 'HOME' ENTERED AT 14:53:13 ON 06 APR 2004)

     FILE 'HCAPLUS' ENTERED AT 14:53:21 ON 06 APR 2004
L1           19 S GUIMOND M?/AU
L2            5 S MOLFINO N?/AU
L3         1784 S ROY D?/AU
L4         1805 S L1-3
L5            3 S L4 AND RHODAMINE
                 SELECT RN L5 2

     FILE 'REGISTRY' ENTERED AT 14:54:53 ON 06 APR 2004
L6            6 S E1-6

     FILE 'HCAPLUS' ENTERED AT 14:55:37 ON 06 APR 2004
L7            1 S L6 AND L5
L8        13213 S L6
L9          113 S L8 AND RHODAMINE
L10           1 S L9 AND PHOTODYNAMIC
L11           2 S L9 AND DIAGNOSIS
L12        5474 S L8(L)THU/RL
L13          26 S L9 AND L12
L14          14 S L13 AND PY<2000

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     FILE 'HCAPLUS' ENTERED AT 16:04:54 ON 06 APR 2004
L16           1 S L15
L17           0 S L16 NOT L5

     FILE 'REGISTRY' ENTERED AT 16:05:41 ON 06 APR 2004
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L19           0 S L18
L20       52360 S OC5-C6-C6/ES
L21           0 S L18 SSS SAM SUB=L20
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L23          42 S L22
L24         794 S L22 FUL
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L30        3946 S PHOTODYNAMIC THERAPY+PFT/CT
L31        5182 S "PHOTOSENSITIZERS (PHARMACEUTICAL)"+PFT/CT
L32      162992 S  LYMPHOCYTE+PFT,NT/CT
L33       35145 S "TRANSPLANT AND TRANSPLANTATION"+PFT/CT
L34       59562 S IMMUNITY+PFT,NT/CT
L35       10647 S RHODAMIN?/OBI
L36          23 S  L35 AND L30
L37          12 S L30(L)RHODAMIN?
L38           9 S L37 NOT L29
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L42       45210 S L39

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L54           0 S " BENZOIC ACID, 2-(3,6-DIETHYLAMINO-4,5-DIBROMO-9H-XANTHEN-9-
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L59          31 S L57 AND O=3
L60          17 S L59 AND "4,5-DIBROMO"
L61           4 S " 2-(3,6-DIAMINO-4,5-DIBROMO-9H-XANTHEN-9-YL)"
L62           2 S "4,5-DIBROMO" AND "BIS(DIETHYLAMINO)"
L63           5 S L39 AND BR=2

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L67     1223588 S BR/ELS

     FILE 'HCAPLUS' ENTERED AT 17:06:42 ON 06 APR 2004

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L70          26 S L69 AND N=2
L71          57 S L55 AND "BIS(DIETHYLAMINO)"
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L1            19 S GUIMOND M?/AU
L2             5 S MOLFINO N?/AU
L3          1784 S ROY D?/AU
L4          1805 S L1-3
L5             3 S L4 AND RHODAMINE
               SELECT RN L5 2

     FILE 'REGISTRY' ENTERED AT 14:54:53 ON 06 APR 2004
L6             6 S E1-6

     FILE 'HCAPLUS' ENTERED AT 14:55:37 ON 06 APR 2004
L7             1 S L6 AND L5

=> d ibib abs hitstr ind

L7   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2001:265273  HCAPLUS
DOCUMENT NUMBER:          134:292146
TITLE:                    Rhodamine derivatives for photodynamic
                          diagnosis and treatment
INVENTOR(S):              Roy, Denis-Claude; Guimond, Martin
                          ; Molfino, Nestor A.
PATENT ASSIGNEE(S):       Universite de Montreal, Can.; Hopital
                          Maisonneuve-Rosemont
SOURCE:                   PCT Int. Appl., 60 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.   DATE
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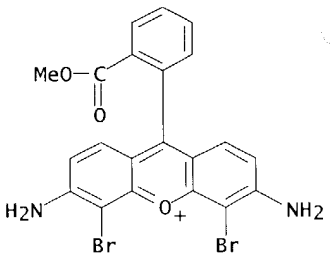
     WO 2001024824      A1   20010412       WO 2000-CA1142    20001003
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     BR 2000014135      A    20020521       BR 2000-14135     20001003
     EP 1267931         A1   20030102       EP 2000-965683    20001003
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
     JP 2003510372      T2   20030318       JP 2001-527823    20001003
PRIORITY APPLN. INFO.:                    US 1999-157790P  P  19991005
                                          WO 2000-CA1142   W  20001003

AB   The present invention relates to the use of the photoactivable derivs. for
     the photodynamic treatment for the selective destruction and/or
     inactivation of immunol. reactive cells without affecting the normal cells
     and without causing systemic toxicity for the patient, wherein appropriate
     intracellular levels of said derivs. are achieved and irradn. of a
     suitable wavelength and intensity is applied.  Examples are given of the
     selective phototoxicity of rhodamine derivs. against K562 cells,
     CEM cells, PHA-activated lymphocytes, activated CD4+ and CD8+ cells and
     human B cells.  Immunol. disorders, including graft-vs-host disease are
     treated with photodynamic therapy.
IT   333957-97-4
     RL: BAC (Biological activity or effector, except adverse); BPR (Biological
```

process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)

RN 333957-97-4 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, bromide (9CI) (CA INDEX NAME)



● Br^-

IT **333957-95-2 333957-96-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)

RN 333957-95-2 HCAPLUS
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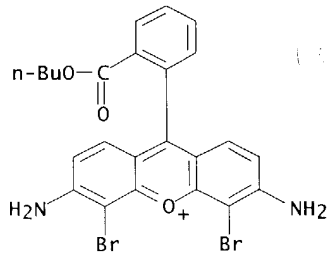

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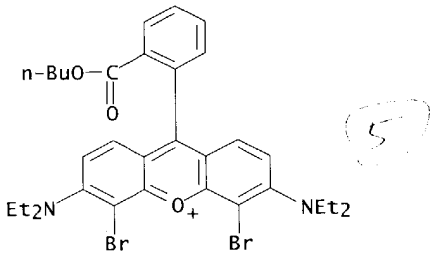

● Cl^-

IT **333957-98-5 333957-99-6**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)
RN 333957-98-5 HCAPLUS
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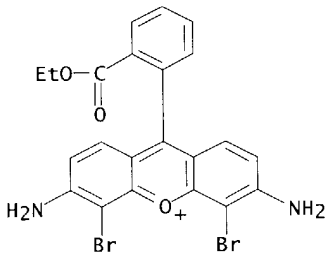

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RN 333957-99-6 HCAPLUS
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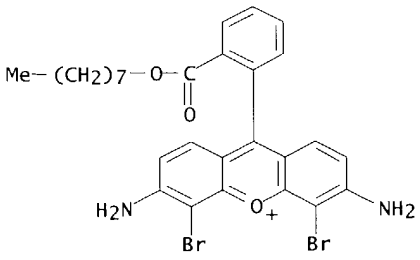


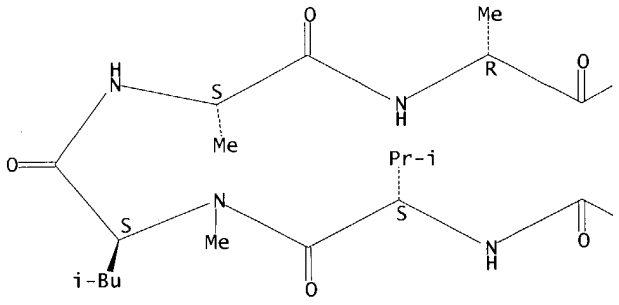
● Br^-

IT **59865-13-3**, Cyclosporin A

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders: effect of cyclosporin A on **rhodamine** cellular efflux)
RN 59865-13-3 HCAPLUS
CN Cyclosporin A (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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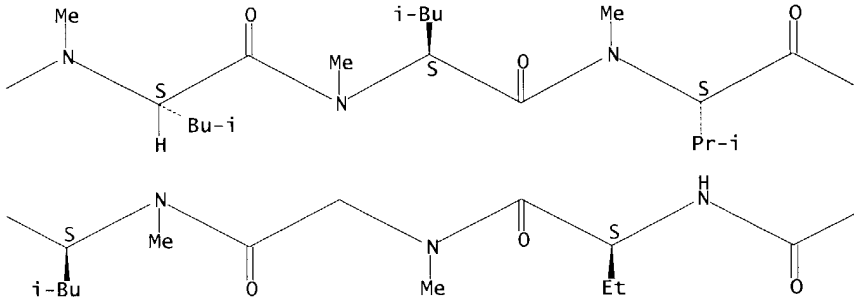

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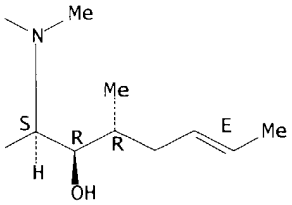

IC ICM A61K041-00
CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 15

ST **rhodamine** deriv immunol disorder photodynamic therapy

IT Lymphocyte
(PHA-activated; **rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders: phototoxicity against immunol. reactive cells)

IT Immunity
(disorder; **rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)

IT Cytometry
(flow; photoactivatable **rhodamine** derivs. for evaluating transport mechanism of cells by flow cytometry)

IT Transplant and Transplantation
(graft-vs.-host reaction; **rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)

IT Allergy
Autoimmune disease
Diagnosis
Photodynamic therapy
Photosensitizers (pharmaceutical)
Transplant rejection
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)

IT B cell (lymphocyte)
CD4-positive T cell
CD8-positive T cell
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders: phototoxicity against immunol. reactive cells)

IT Bone marrow
Hematopoietic precursor cell
Mononuclear cell (leukocyte)
Transplant and Transplantation
(**rhodamine** derivs. for photodynamic ex vivo treatment of hematopoietic cells)

IT **333957-97-4**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)

IT **333957-95-2 333957-96-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)

IT **333957-98-5 333957-99-6**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders)

IT **59865-13-3**, Cyclosporin A
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(**rhodamine** derivs. for photodynamic diagnosis and treatment of immunol. disorders: effect of cyclosporin A on **rhodamine** cellular efflux)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L22             STR
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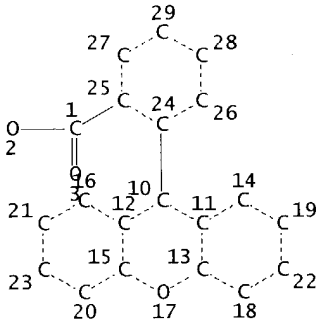

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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS  23

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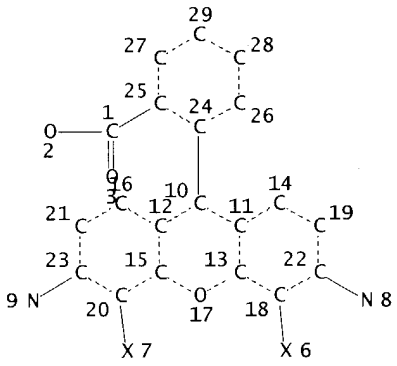

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L29           24 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L28


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L29  ANSWER 1 OF 24  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2003:749309  HCAPLUS
DOCUMENT NUMBER:          140:213073
TITLE:                    Ca2+-dependent and caspase-3-independent apoptosis
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caused by damage in Golgi apparatus due to 2,4,5,7-tetrabromorhodamine 123 bromide-induced photodynamic effects

AUTHOR(S): Ogata, Maiko; Inanami, Osamu; Nakajima, Mihoko; Nakajima, Takayuki; Hiraoka, Wakako; Kuwabara, Mikinori

CORPORATE SOURCE: Laboratory of Radiation Biology, Department of Environmental Veterinary Science, Graduate School of Veterinary Medicine, Hokkaido University, Sapporo, Japan

SOURCE: Photochemistry and Photobiology (2003), 78(3), 241-247
CODEN: PHCBAP; ISSN: 0031-8655

PUBLISHER: American Society for Photobiology

DOCUMENT TYPE: Journal

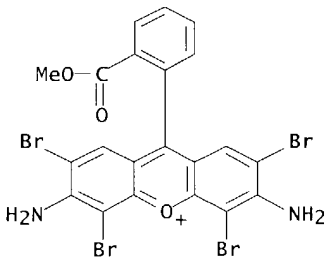
LANGUAGE: English

AB To clarify the role of the Golgi app. in photodynamic therapy-induced apoptosis, its signaling pathway was studied after photodynamic treatment of human cervix carcinoma cell line HeLa, in which a photosensitizer, 2,4,5,7-tetrabromorhodamine 123 bromide (TBR), was incorporated into the Golgi app. Laser scanning microscopic anal. of TBR-loaded HeLa cells confirmed that TBR was exclusively located in the Golgi app. HeLa cells incubated with TBR for 1 h were then exposed to visible light using an Xe lamp. Light of wavelength below 670 nm was eliminated with a filter. Morphol. observation of nuclei stained with Hoechst 33342 revealed that apoptosis of cells was induced by exposure to light. ESR spectrometry showed that light-exposed TBR produced both singlet oxygen (1O2) and superoxide anion (O2-). Apoptosis induction by TBR was inhibited by pyrrolidine dithiocarbamate, an O2- scavenger, but not by NaN3, a quencher of 1O2. Furthermore, TBR-induced apoptosis was inhibited by aurintricarboxylic acid and ZnCl2, which are known as inhibitors of DNase (DNase) .gamma., and (acetoxymethyl)-1,2-bis(o-aminophenoxy)-ethane-N,N,N',N'-tetraacetic acid, a chelator of Ca2+, but not by acetyl Asp-Glu-Val-Asp-aldehyde, an inhibitor of caspase-3. These results suggested that O2- was responsible for TBR-induced apoptosis, and Ca2+-dependent and caspase-3-independent nuclease such as DNase .gamma. played an important role in apoptotic signaling triggered by Golgi dysfunction.

IT **623903-26-4**, Tetrabromorhodamine 123
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tetrabromorhodamine 123; Golgi app., calcium, caspase, and DNase role in PDT-induced apoptosis in cervical carcinoma)

RN 623903-26-4 HCAPLUS

CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, bromide (9CI) (CA INDEX NAME)



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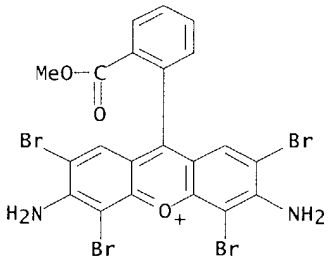
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:226526 HCAPLUS
DOCUMENT NUMBER: 139:377312
TITLE: "Mitochondrial" photochemical drugs do not release toxic amounts of 1O2 within the mitochondrial matrix space
AUTHOR(S): Petrat, Frank; Pindiur, Stanislaw; Kirsch, Michael; de Groot, Herbert
CORPORATE SOURCE: Institut fur Physiologische Chemie, Universitaetsklinikum, Essen, D-45122, Germany
SOURCE: Archives of Biochemistry and Biophysics (2003), 412(2), 207-215
CODEN: ABBIA4; ISSN: 0003-9861
PUBLISHER: Elsevier Science
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Previously, we demonstrated that mitochondrial NAD(P)H is the primary target of singlet oxygen (1O2) generated by photoactivation of mitochondria-selective rhodamine derivs. Hence, local NAD(P)H oxidn./fluorescence decrease may be used to reveal the site of intracellular 1O2 generation. Therefore, in addn. to the previously used tetramethylrhodamine methylester (TMRM), 2',4',5',7'-tetrabromorhodamine 123 bromide (TBRB) and rhodamine 123 (Rho 123), we tested here whether mitochondrial NAD(P)H of cultured hepatocytes is directly oxidized upon irradn. of different "mitochondrial" photosensitizers (Photofrin; protoporphyrin IX; Al(III) phthalocyanine chloride tetrasulfonic acid; meso-tetra(4-sulfonatophenyl)porphine dihydrochloride; Visudyne). In contrast to TMRM and Rho 123, which directly oxidized NAD(P)H upon irradn., irradn. of intracellular TBRB and the photochem. drugs only indirectly affected mitochondrial NAD(P)H due to loss of mitochondrial integrity. In line with this result only TMRM and Rho 123 exclusively localized within the mitochondrial matrix. Due to these results it is doubtful whether real mitochondrial photosensitizers actually exist among the photochem. drugs applicable/used for photodynamic therapy.

IT **623903-26-4**
RL: PAC (Pharmacological activity); BIOL (Biological study)
(mitochondrial PDT photosensitizers do not release toxic amts. of 1O2 within mitochondrial matrix space)
RN 623903-26-4 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, bromide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:777919 HCAPLUS
DOCUMENT NUMBER: 137:280622

TITLE: Halogenated rhodamine dye derivatives and their therapeutic applications
INVENTOR(S): Habi, Abdelkrim; Gravel, Denis; Villeneuve, Luc; Forte, Jean-Pierre; Su, Hongsheng; Vaillancourt, Marc
PATENT ASSIGNEE(S): Theratechnologies Inc., Can.
SOURCE: PCT Int. Appl., 117 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002079183	A1	20021010	WO 2002-CA438	20020327
WO 2002079183	C1	20030220		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1276734	A1	20030122	EP 2002-708105	20020327
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002004489	A	20030401	BR 2002-4489	20020327
US 2003212126	A1	20031113	US 2003-297088	20030530

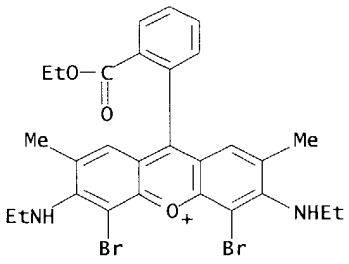
PRIORITY APPLN. INFO.:
CA 2001-2342675 A 20010402
US 2001-822223 A 20010402
WO 2002-CA438 W 20020327

OTHER SOURCE(S): MARPAT 137:280622

AB Bromo derivs. of rhodamine 110, rhodamine B, and rhodamine 6G and other halo rhodamine derivs. are useful as intermediates and as bactericides and antiviral agents and in the treatment of immunol. disorders. In an example, rhodamine B Me ester was dihydrogenated and then brominated and oxidized and treated with acetic acid to provide the purple acetate salt of 2,7-dibromorhodamine B Me ester.

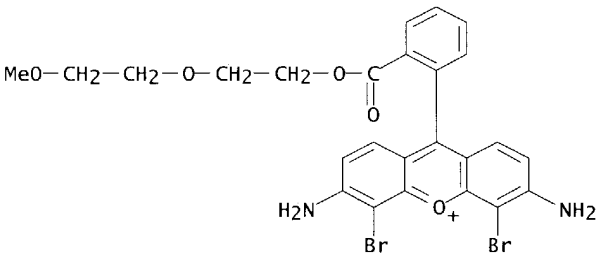
IT **467232-05-9P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(green-red dye; prodn. of halogenated rhodamine dye derivs. and their therapeutic applications)

RN 467232-05-9 HCAPLUS
CN Xanthylium, 4,5-dibromo-9-[2-(ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-dimethyl-, bromide (9CI) (CA INDEX NAME)



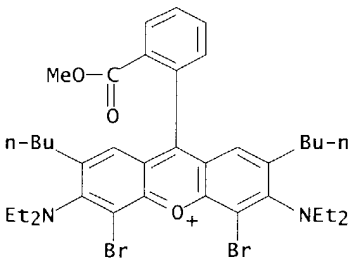
● Br^-

IT **467232-07-1P 467232-23-1P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(red dye; prodn. of halogenated rhodamine dye derivs. and their therapeutic applications)
RN 467232-07-1 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-[[2-(2-methoxyethoxy)ethoxy]carbonyl]phenyl]-, bromide (9CI) (CA INDEX NAME)



● Br^-

RN 467232-23-1 HCAPLUS
CN Xanthylium, 4,5-dibromo-2,7-dibutyl-3,6-bis(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-, bromide (9CI) (CA INDEX NAME)



● Br^-

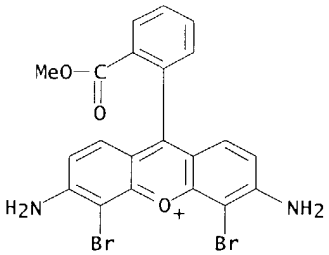
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:541337 HCAPLUS
DOCUMENT NUMBER: 137:167817
TITLE: P-glycoprotein targeting: a unique strategy to selectively eliminate immunoreactive T cells
AUTHOR(S): Guimond, Martin; Balassy, Antonia; Barrette, Melanie; Brochu, Sylvie; Perreault, Claude; Roy, Denis Claude
CORPORATE SOURCE: Division of Hematology-Immunology, Maisonneuve-Rosemont Hospital Research Center, Department of Medicine, Universite de Montreal, Montreal, QC, Can.
SOURCE: Blood (2002), 100(2), 375-382
CODEN: BLOOAW; ISSN: 0006-4971
PUBLISHER: American Society of Hematology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB T lymphocytes have been found to harbor P-glycoprotein (Pgp) and to demonstrate modulation of its ion channel transporter function according to the state of activation of T lymphocytes. We hypothesized that cytotoxic chems. that are extruded by Pgp could be used to specifically eliminate immunoreactive T-cell populations. In this study, we evaluated the capacity of 4,5-dibromorhodamine Me ester (TH9402), a photosensitizer structurally similar to rhodamine, a dye transported by Pgp, and which becomes highly cytotoxic on activation with visible light to selectively deplete alloreactive T lymphocytes. Stimulation of T cells with mitogens or allogeneic major histocompatibility complex-mismatched cells resulted in the preferential retention of the TH9402 rhodamine-deriv. in activated T cells, both CD4+ and CD8+. Photodynamic cell therapy of TH9402-exposed T cells led to the selective elimination of immunoreactive T-cell populations. In addn., this treatment preserved resting T cells and their capacity to respond to third-party cells. Inhibition of Pgp enhanced cellular trapping of the dye in nonactivated T cells and resulted in their depletion after exposure to light. Targeting of Pgp-deficient cells may therefore represent an appealing strategy for the prevention and treatment of graft-vs.-host disease and other alloimmune or autoimmune disorders.

IT **174230-05-8**, TH9402
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(P-glycoprotein targeting to selectively eliminate immunoreactive T cells)

RN 174230-05-8 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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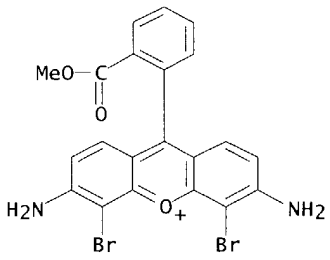
REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:335895 HCAPLUS
DOCUMENT NUMBER: 137:75306
TITLE: Prevention of graft-versus-host disease while preserving graft-versus-leukemia effect after selective depletion of host-reactive T cells by photodynamic cell purging process
AUTHOR(S): Chen, Benny J.; Cui, Xiuyu; Liu, Congxiao; Chao, Nelson J.
CORPORATE SOURCE: Bone Marrow Transplantation Program, Duke University Medical Center, Durham, NC, 27705, USA
SOURCE: Blood (2002), 99(9), 3083-3088
CODEN: BLOOAW; ISSN: 0006-4971
PUBLISHER: American Society of Hematology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In this study, we investigated the possibility of selective depletion of donor alloantigen-specific T cells from C57BL/6 (H-2b) mice to prevent graft-vs.-host disease (GVHD). These cells were first activated with irradiated BALB/c (H-2d) host spleen cells in a 5-day mixed lymphocyte culture. Following this activation, a photoactive rhodamine deriv. called 4,5-dibromorhodamine 123 (TH9402), was added. This compd. is selectively retained in the mitochondria of activated host-reactive cells but not tumor-or third-party-specific resting cells. The treated cells were subsequently exposed to visible light (514 nm) to deplete the TH9402-enriched activated host-reactive cells. Treatment with photodynamic cell purging process (PDP) inhibited antihost responses measured by cytotoxic T lymphocytes (CTL) by 93%, and interferon-.gamma. prodn. by 66%. By contrast, anti-BCL1 (BALB/c-origin leukemia/lymphoma) and anti-third-party C3H/HeJ (H-2k) responses were preserved. PDP-treated primed C57BL/6 cells were further tested in vivo. All lethally irradiated BALB/c mice inoculated with BCL1 cells and T-cell-depleted bone marrow cells developed leukemia by day +30, with 50% mortality by 100 days. All mice died of GVHD after addn. of 5 .times. 106 untreated primed C57BL/6 cells. However, addn. of same nos. of PDP-treated cells allowed 90% of the recipients to survive more than 100 days without detectable BCL1 tumor cells and free of GVHD. Moreover, PDP-treated primed C57BL/6 cells retained the ability to induce GVHD in the third-party C3H/HeJ mice. These data suggest that PDP can selectively deplete host alloantigen-specific T cells for GVHD prevention and immune and antileukemia function preserve.
IT **174230-05-8**, TH9402
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prevention of graft-vs.-host disease while preserving graft-vs.-leukemia effect after selective depletion of host-reactive T cells by photodynamic cell purging)
RN 174230-05-8 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:265273 HCAPLUS
DOCUMENT NUMBER: 134:292146
TITLE: Rhodamine derivatives for photodynamic diagnosis and treatment
INVENTOR(S): Roy, Denis-Claude; Guimond, Martin; Molfino, Nestor A.
PATENT ASSIGNEE(S): Universite de Montreal, Can.; Hopital Maisonneuve-Rosemont
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001024824	A1	20010412	WO 2000-CA1142	20001003
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000014135	A	20020521	BR 2000-14135	20001003
EP 1267931	A1	20030102	EP 2000-965683	20001003
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003510372	T2	20030318	JP 2001-527823	20001003

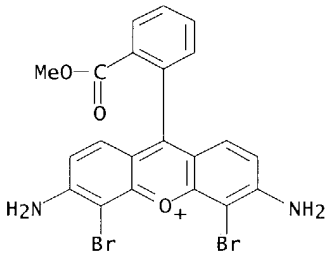
PRIORITY APPLN. INFO.: US 1999-157790P P 19991005
WO 2000-CA1142 W 20001003

AB The present invention relates to the use of the photoactivable derivs. for the photodynamic treatment for the selective destruction and/or inactivation of immunol. reactive cells without affecting the normal cells and without causing systemic toxicity for the patient, wherein appropriate intracellular levels of said derivs. are achieved and irradn. of a suitable wavelength and intensity is applied. Examples are given of the selective phototoxicity of rhodamine derivs. against K562 cells, CEM cells, PHA-activated lymphocytes, activated CD4+ and CD8+ cells and human B cells. Immunol. disorders, including graft-vs-host disease are treated with photodynamic therapy.

IT **333957-97-4**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological

process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(rhodamine derivs. for photodynamic diagnosis and treatment of immunol. disorders)

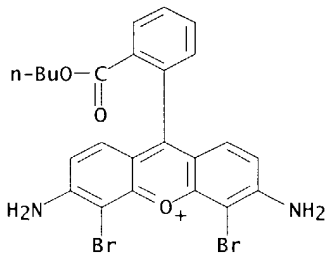
RN 333957-97-4 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, bromide (9CI) (CA INDEX NAME)



● Br⁻

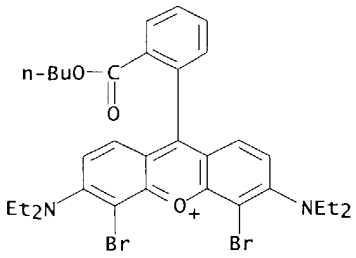
IT **333957-95-2 333957-96-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(rhodamine derivs. for photodynamic diagnosis and treatment of immunol. disorders)

RN 333957-95-2 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(butoxycarbonyl)phenyl]-, bromide (9CI) (CA INDEX NAME)



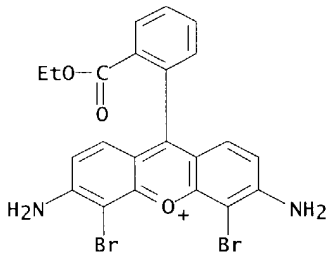
● Br⁻

RN 333957-96-3 HCAPLUS
CN Xanthylium, 4,5-dibromo-9-[2-(butoxycarbonyl)phenyl]-3,6-bis(diethylamino)-, chloride (9CI) (CA INDEX NAME)



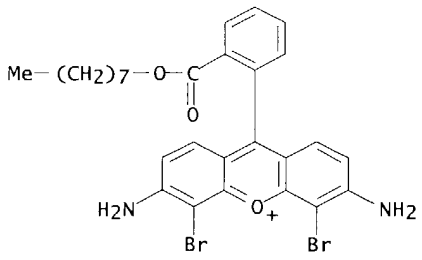
● Cl⁻

IT **333957-98-5 333957-99-6**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(rhodamine derivs. for photodynamic diagnosis and treatment of immunol. disorders)
RN 333957-98-5 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(ethoxycarbonyl)phenyl]-, bromide (9CI) (CA INDEX NAME)



● Br⁻

RN 333957-99-6 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-[(octyloxy)carbonyl]phenyl]-, bromide (9CI) (CA INDEX NAME)



● Br⁻

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS

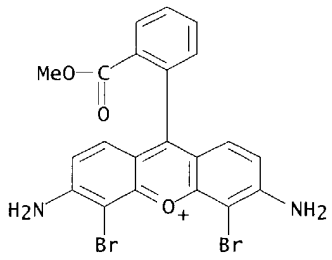
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:20398 HCAPLUS
DOCUMENT NUMBER: 134:204394
TITLE: Eradication of multiple myeloma and breast cancer cells by TH9402-mediated photodynamic therapy: implication for clinical ex vivo purging of autologous stem cell transplants
AUTHOR(S): Brasseur, N.; Menard, I.; Forget, A.; El Jastimi, R.; Hamel, R.; Molfino, N. A.; Van Lier, J. E.
CORPORATE SOURCE: Department of Nuclear Medicine and Radiobiology, Faculty of Medicine, Universite de Sherbrooke, Sherbrooke, QC, J1H 5N4, Can.
SOURCE: Photochemistry and Photobiology (2000), 72(6), 780-787
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB High-dose chemotherapy combined with autologous transplantation using bone marrow or peripheral blood-derived stem cells (PBSC) is now widely used in the treatment of hematol. malignancies as well as some solid tumors like breast cancer (BC). However, some controversial results were recently obtained in the latter case. The presence of malignant cells in the autograft has been assocd. with the recurrence of the disease, and purging procedures are needed to eliminate this risk. The aim of this study was to evaluate the potential of the photosensitizer 4,5-dibromorhodamine Me ester (TH9402), a dibrominated rhodamine deriv., to eradicate multiple myeloma (MM) and BC cell lines, while sparing more than 50% of normal pluripotential blood stem cells from healthy volunteers. The human BC MCF-7 and T-47D and MM RPMI 8226 and NCI-H929 cell lines were used to optimize the photodynamic purging process. Cell concn. and the cell suspension thickness as well as the dye and light doses were varied in order to eventually treat 1-2 L of apheresis. The light source consisted of two fluorescent scanning tubes emitting green light centered about 515 nm. The cellular uptake of TH9402 was measured during the incubation and washout periods and after photodynamic treatment (PDT) using spectrofluorometric anal. The limiting diln. assay showed that an eradication rate of more than 5 logs is obtained when using a 40 min incubation with 5-10 .mu.M dye followed by a 90 min washout period and a light dose of 5-10 J/cm2 (2.8 mW/cm2) in all cell lines. Agitating the 2 cm thick cell suspension contg. 20 .times. 106 cells/mL during PDT was essential for maximal photoinactivation. Expts. on mobilized PBSC obtained from healthy volunteers showed that even more drastic purging conditions than those found optimal for maximal eradication of the malignant cell lines were compatible with a good recovery of hematopoietic progenitors cells. The absence of significant toxicity towards normal hematopoietic stem cells, combined with the 5 logs eradication of cancer cell lines induced by this procedure suggests that TH9402 offers an excellent potential as an ex vivo photodynamic purging agent for autologous transplantation in MM and BC treatment.

IT **174230-05-8**, TH9402
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(myeloma and breast cancer cells eradication by TH9402-mediated photodynamic therapy: implication for clin. ex vivo purging of autologous stem cell transplants)

RN 174230-05-8 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

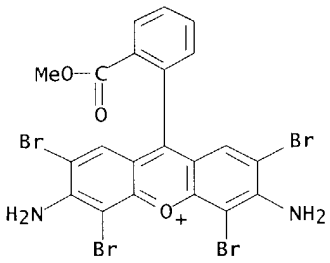
L29 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:911534 HCAPLUS
DOCUMENT NUMBER: 134:66121
TITLE: Compositions and methods for assaying subcellular conditions and processes using energy transfer for drug screening
INVENTOR(S): Dykens, James A.; Velicelebi, Gonul; Ghosh, Soumitra S.
PATENT ASSIGNEE(S): Mitokor, USA
SOURCE: PCT Int. Appl., 189 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000079274	A2	20001228	WO 2000-US17380	20000622
WO 2000079274	A3	20020110		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6323039	B1	20011127	US 1999-338122	19990622
US 6280981	B1	20010828	US 2000-514569	20000223
EP 1210596	A2	20020605	EP 2000-943119	20000622
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003506014	T2	20030218	JP 2001-505191	20000622

PRIORITY APPLN. INFO.:
US 1999-140433P P 19990622
US 1999-338122 A 19990622
US 2000-176383P P 20000114
WO 2000-US17380 W 20000622

AB The invention provides compns. and methods for monitoring subcellular compartments such as organelles by energy transfer techniques that do not require specific intermol. affinity binding events between energy transfer donor and energy transfer acceptor mols. pH. Provided are methods for assaying cellular membrane potential, including mitochondrial membrane potential, by energy transfer methodologies including fluorescence resonance energy transfer (FRET). Diagnostic and drug screening assays

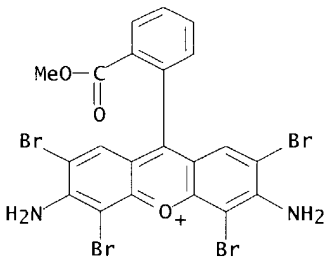
are also provided.
IT **83796-96-7**, Tetrabromo-rhodamine 123
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(tetrabromorhodamine 123; compns. and methods for assaying subcellular conditions and processes using energy transfer for drug screening)
RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L29 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:507144 HCAPLUS
DOCUMENT NUMBER: 133:360498
TITLE: Nonthermal ureteral tissue bonding: comparison of photochemical collagen crosslinking with thermal laser bonding
AUTHOR(S): Merguerian, Paul A. M. D.; Pugach, Jeff L. M. D.; Lilge, Lothar D.
CORPORATE SOURCE: Urology Div., Hospital for Sick Children, Univ. of Toronto, Toronto, ON, Can.
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1999), 3590(Lasers in Surgery: Advanced Characterization, Therapeutics, and Systems IX), 194-202
CODEN: PSISDG; ISSN: 0277-786X
PUBLISHER: SPIE-The International Society for Optical Engineering
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Because of difficulties with suture placement during minimally invasive procedures, many have sought alternative methods of creating tissue anastomoses. Although well studied, thermal laser tissue bonding has the potential of causing collateral thermal injury. Non-thermal tissue bonding agents, which cross-link proteins when activated with light, are currently being explored. We recently reported successful non-thermal bonding using tetrabromorhodamine (TBR). The bond was stronger than sutured repairs but weaker than laser thermal bonding. We currently report our ex-vivo experience with an alternate agent, riboflavin-5-phosphate and compare these results to thermal bonding and TBR. Successful ex vivo photochem. tissue welding with riboflavin of the rabbit ureter was achieved, without the generation of heat. Bon strength similar to that obtained with thermal welding was achieved.
IT **83796-96-7**, Tetrabromo-rhodamine 123
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(nonthermal ureteral tissue bonding: comparison of photochem. collagen crosslinking with thermal laser bonding)
RN 83796-96-7 HCAPLUS

CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



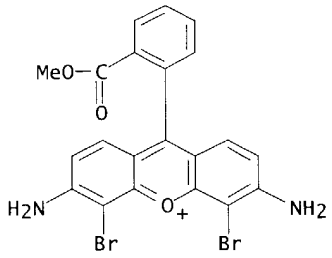
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:570227 HCAPLUS
DOCUMENT NUMBER: 131:308414
TITLE: Ex vivo photodynamic purging in chronic myelogenous leukemia and other neoplasias with rhodamine derivatives
AUTHOR(S): Villeneuve, Luc
CORPORATE SOURCE: Theratechnologies Inc., Montreal, QC, H3B 1S6, Can.
SOURCE: Biotechnology and Applied Biochemistry (1999), 30(1), 1-17
CODEN: BABIEC; ISSN: 0885-4513
PUBLISHER: Portland Press Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 294 refs. Photodynamic therapy (PDT), a cancer treatment already used early in this century, has distinctive advantages over conventional chemotherapy, namely its often obsd. preferential accumulation in cancer cells and its low intrinsic toxicity. Aggressive therapeutic modalities using high doses of chemotherapy and/or radiation therapy are now commonplace treatments for leukemia, lymphoma and various non-haematol. malignancies. These intensive approaches have often been used in assocn. with hematopoietic-progenitor-cell support and have induced major responses and remissions in patients with relapsed and refractory diseases, ultimately contributing to improve the disease-free survival of patients with high risk. This has encouraged Theratechnologies, a Montreal-based pharmaceutical company, to develop photodynamic ex vivo purging procedures, including the development of new photosensitizers and irradn. devices for the safe eradication of neoplastic cells from autologous grafts. Our first specific objective, therefore, was to design, synthesize, purify and test photoactive rhodamine derivs. 4,5-Dibromorhodamine 123 (TH9402), a gas and phosphorus coating characteristic of an efficient scanning fluorescent source for extra-corporeal PDT using rhodamine derivs., was selected because of its photophys. properties, low toxicity and stability. TH9402 photodynamic-cell-therapy process conditions recognized as safe for normal human haematopoietic stem cells and progenitors demonstrated the efficacy of the purging procedure on various leukemias (including chronic-myelogenous-leukemia) as well as non-Hodgkin-leukemias and metastatic-breast-cancer cell lines.

IT **174230-05-8**, TH 9402
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(TH 9402; ex vivo photodynamic purging in chronic myelogenous leukemia and other neoplasias with rhodamine derivs.)

RN 174230-05-8 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 292 THERE ARE 292 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:244672 HCAPLUS
DOCUMENT NUMBER: 130:277634
TITLE: Screening for oligonucleotide inhibitors of gene expression using conjugates with activatable reactive substances
INVENTOR(S): Prescott, Catherine Denise
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

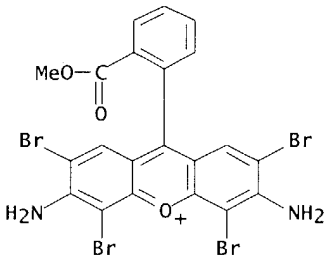
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9918116	A1	19990415	WO 1998-US21052	19981007
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1023312	A1	20000802	EP 1998-952108	19981007
R: BE, CH, DE, DK, FR, GB, IT, LI, NL				
JP 2001519141	T2	20011023	JP 2000-514925	19981007
US 6387703	B1	20020514	US 2000-529095	20000406

PRIORITY APPLN. INFO.: US 1997-61218P P 19971007
WO 1998-US21052 W 19981007

AB A method of screening for compds., particularly oligonucleotides, that modulate gene expression, particularly those which lower gene expression is described. The method uses a conjugate of the oligonucleotide and an activatable reactive group, such as a photosensitizing dye, preferably a compd. that generates reactive oxygen species. Target cells are incubated with the conjugate and the reactive group is activated and the effect on gene expression is assayed.

IT **83796-96-7D**, Tetrabromo-rhodamine 123, derivs., conjugates with oligonucleotides
RL: BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(tetrabromorhodamine 123, photoactivatable inhibition of gene expression using; screening for oligonucleotide inhibitors of gene expression using conjugates with activatable reactive substances)

RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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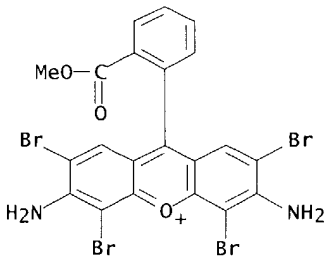
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:298888 HCAPLUS
DOCUMENT NUMBER: 129:51463
TITLE: [125I/127I/131I]Iodorhodamine: Synthesis, Cellular Localization, and Biodistribution in Athymic Mice Bearing Human Tumor Xenografts and Comparison with [99mTc]Hexakis(2-methoxyisobutylisonitrile)
AUTHOR(S): Harapanhalli, Ravi S.; Roy, Aloka M.; Adelstein, S. James; Kassis, Amin I.
CORPORATE SOURCE: Department of Radiology (Nuclear Medicine), Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Journal of Medicinal Chemistry (1998), 41(12), 2111-2117
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of halogenated rhodamine (Rh) derivs. was carried out by controlling the stoichiometry of the halogenating agents, bromine and iodine monochloride. In the no-carrier-added synthesis of radioiodinated rhodamine 123, direct labeling of rhodamine 123 (Rh 123) with Na125I/Na131I required the presence of the oxidant peracetic acid. 125I/131I-Rh 123 was synthesized in modest yields (40-45%). HPLC purifn. sepd. Rh 123 from its mono- and diiodo derivs. Monohalogenation of Rh 123 did not alter the compd.'s ability to permeate viable cells and localize in mitochondria. 125I/131I-Rh 123 was stable in serum in vitro but rapidly metabolized after i.v. injection into mice. Consequently, scintigraphy and biodistribution data reveal poor targeting of s.c. growing human tumor xenografts. The results are compared to those obtained following the administration of [99mTc]hexakis(2-methoxyisobutylisonitrile) which also did not image human tumor xenografts in nude mice.
IT **83796-96-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and biodistribution of radioiodinated rhodamine 123 in tumor imaging)
RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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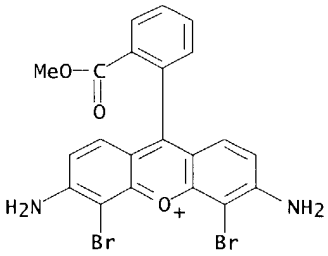
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:104125 HCAPLUS
DOCUMENT NUMBER: 126:183387
TITLE: Spectroscopic and photophysical investigations on the nature of localization of rhodamine-123 and its dibromo derivative in different cell lines
AUTHOR(S): Villeneuve, Luc; Pal, Prabir; Durocher, Gilles; Migneault, David; Girard, Denis; Giasson, Richard; Balassy, Antonia; Blanchard, Louise; Gaboury, Louis
CORPORATE SOURCE: Laboratoire de pathologie moleculaire, Departement de pathologie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.
SOURCE: Journal of Fluorescence (1996), 6(4), 209-219
CODEN: JOFLEN; ISSN: 1053-0509
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Steady-state and time-resolved spectroscopic properties of rhodamine-123 (rh123) and 4,5-dibromorhodamine Me ester (dbr123) bound to different cell lines are evaluated. Studies are also performed on the dye bound to extd. mitochondria. Results are compared with those obtained in homogeneous and microheterogeneous media. Results suggest that these dyes can specifically bind only with cell mitochondria. As a result of binding, excitation and emission spectra are red shifted by 10 to 12 nm. The fluorescence decay of these dyes bound to mitochondria shows two lifetimes. Values are about 4.0 and 2.0 ns for rh123 and about 1.9 and 0.5 ns for dbr123. Detailed global anal. of emission wavelength and dye concn. dependences of the fluorescence decay is performed. Results indicate that these dyes are bound to two different binding sites at mitochondria. The decay-assocd. fluorescence spectrum for the species corresponding to each binding site is recovered. Species 1, corresponding to the longer lifetime, is found to be more red shifted compared to species 2. The fluorescence of species 2 is heavily quenched. The origin of this quenching is explained in terms of resonance energy transfer between donor species 2 and acceptor species 1. The possible nature of the two binding sites is also discussed.

IT **174230-05-8**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (spectroscopic and photophys. investigations on the nature of localization of rhodamine-123 and its dibromo deriv. in different cell lines)

RN 174230-05-8 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)

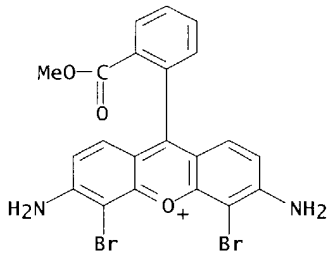


L29 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:538169 HCAPLUS
DOCUMENT NUMBER: 125:260967
TITLE: Spectroscopic and photophysical properties of some new rhodamine derivatives in cationic, anionic and neutral micelles
AUTHOR(S): Pal, P.; Zeng, H.; Durocher, G.; Girard, D.; Giasson, R.; Blanchard, L.; Gaboury, L.; Villeneuve, L.
CORPORATE SOURCE: Laboratoire de photophysique moleculaire, Departement de chimie, Universite de Montreal, C.P. 6128, Succ. Centre-ville, Montreal, Que., H3C 3J7, Can.
SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (1996), 98(1-2), 65-72
CODEN: JPPCEJ; ISSN: 1010-6030
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The spectroscopic and photophys. characterization of rhodamine 123 (dye 1), 4,5-dibromorhodamine Me ester (dye 2) and 4,5-dibromorhodamine Bu ester (dye 3) are reported in homogeneous media like water and some alcs. and also in microheterogeneous media; anionic sodium dodecylsulfate (SDS), cationic cetyltrimethylammonium bromide (CTAB) and neutral triton X-100 (TX) micelles. The selective biodistribution of these ionic drugs in tissues and membranes strongly influence their photosensitizing properties which have been part of our earlier studies. Results suggest that the hydrogen bonding capability of the amino end group lone pair of these dyes dominates in water. All these dyes interact with anionic SDS micelles. The interaction is mainly electrostatic in nature. At low SDS concns. (below c.m.c.), dye-SDS aggregate formation takes place. But above c.m.c. only the monomeric dye form is obsd. The penetration of dye 3 in SDS is a little less compared to dyes 1 and 2. Dyes 2 and 3 show a finite interaction with CTAB micelle unlike dye 1. With neutral TX micelles all the dyes form strong complexes. The fluorescence quantum yield (.PHI.F) of these three dyes in TX is lower. In time-resolved fluorescence expts., two lifetimes are obsd. The effects of the TX concn. on the fluorescence decay are measured. The decay assocd. spectra of dye 2 in TX are obtained by global compartmental anal. The dye-surfactant interaction mechanisms are also discussed.

IT **174230-05-8 174230-06-9**
RL: PRP (Properties)
(spectroscopic and photophys. properties of rhodamine derivs. in homogeneous media and micelles)

RN 174230-05-8 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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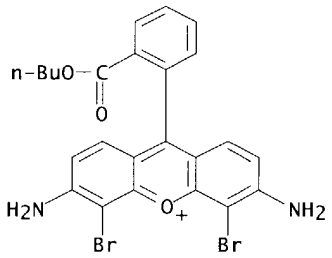
RN 174230-06-9 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(butoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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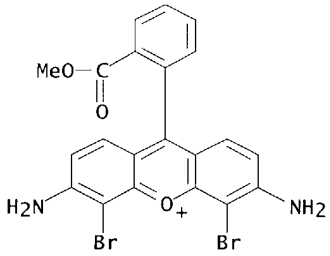
L29 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:96151 HCAPLUS
DOCUMENT NUMBER: 124:197239
TITLE: Phototoxicity of some bromine-substituted rhodamine dyes: synthesis, photophysical properties and application as photosensitizers
AUTHOR(S): Pal, PRabir; Zeng, Hualing; Durocher, Gilles; Girard, Denis; Li, Tiechao; Gupta, Ajay K.; Giasson, Richard; Blanchard, Louise; Gaboury, Louis; et al.
CORPORATE SOURCE: Lab. Photophys. Mol., Univ. Montreal, Montreal, QC, Can.
SOURCE: Photochemistry and Photobiology (1996), 63(2), 161-8
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of some bromine-substituted rhodamine derivs., viz., 4,5-dibromorhodamine Me ester (dye 2) and 4,5-dibromorhodamine Bu ester (dye 3), are reported. These dyes were synthesized to promote a more efficient cancer cell photosensitizer for potential use in in vitro bone marrow purging in prepn. for autologous bone marrow transplantation. Spectroscopic and photophys. characterization of these dyes together with rhodamine 123 (dye 1) are reported in water, methanol, ethanol and also in a microheterogeneous system, sodium dodecyl sulfate. The possible mechanism of photosensitization os characterized in terms of singlet oxygen efficiency of these dyes. Singlet oxygen quantum yields for

bromine-substituted dyes are in the range of 0.3-0.5 depending on the solvent. For dye 1 no singlet oxygen prodn. is found. The photodynamic actions of these dyes in different cell lines are tested. It was found that dye 2 and dye 3 are efficient photosensitizers and mediate eradication of K562, EM2, myeloid cell lines (CML) and the SMF-AI rhabdomyosarcoma line.

IT **174230-05-8P 174230-06-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phototoxicity of some bromine-substituted rhodamine dyes: synthesis, photophys. properties and application in leukemia photosensitizations with laser radiation)

RN 174230-05-8 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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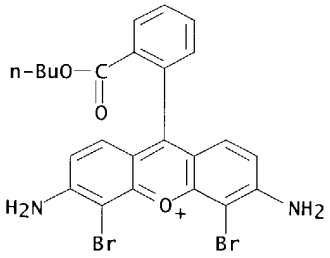
RN 174230-06-9 HCAPLUS
CN Xanthylium, 3,6-diamino-4,5-dibromo-9-[2-(butoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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L29 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:709283 HCAPLUS
DOCUMENT NUMBER: 123:164113
TITLE: DMSO affects the efficiency of photolabeling of tetrabrominated rhodamine to collagen fibers.
AUTHOR(S): Jacques, Steven L.; Awazu, Kunio; Hasan, Tayyaba
CORPORATE SOURCE: M. D. Anderson Cancer Center, Univ. Texas, Houston, TX, 77030, USA

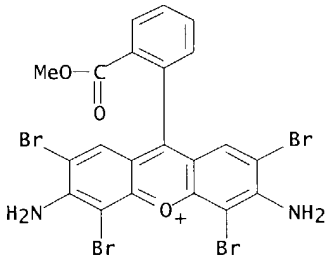
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1995), 2391(Laser-Tissue Interaction VI), 232-7
CODEN: PSISDG; ISSN: 0277-786X
PUBLISHER: SPIE-The International Society for Optical Engineering
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The ability to photolabel a compd., tetrabrominated rhodamine (TBR), onto collagen gels was tested. The influence of DMSO on the efficiency of photolabeling was detd. DMSO enhances the photolabeling presumably by allowing TBR to become more closely assocd. to the collagen fibers such that upon photon absorption which causes debromination to yield a radical, the radical can covalently link to the collagen.

IT **83796-96-7**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(DMSO affects the efficiency of photolabeling of tetrabrominated rhodamine to collagen fibers)

RN 83796-96-7 HCAPLUS

CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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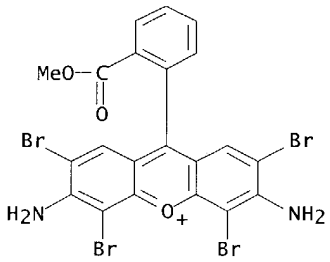
L29 ANSWER 17 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:583719 HCAPLUS
DOCUMENT NUMBER: 123:78614
TITLE: Photodynamic therapy with cationic photosensitizers
AUTHOR(S): Kessel, David; Woodburn, Kathryn; Chang, Ck; Henderson, Bw
CORPORATE SOURCE: Department Pharmacology, Wayne State University School Medicine, Detroit, MI, USA
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1995), 2371, 334-8
CODEN: PSISDG; ISSN: 0277-786X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We characterized sites of photodamage catalyzed by two cationic photosensitizers, tetrabromo-rhodamine 123 (TBR), which is recognized by the multidrug transporter, and a monocationic porphyrin (MCP) which is not. The transporter is an outward transport system assocd. with examples of drug resistance. Irradn. of multidrug-resistant cells treated with TBR resulted in highly-selective photodamage to the transporter site, while MCP catalyzed nonspecific membrane damage to cells regardless of transporter expression.

IT **83796-96-7**, Tetrabromo-rhodamine 123
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(photodynamic therapy with cationic photosensitizers)

RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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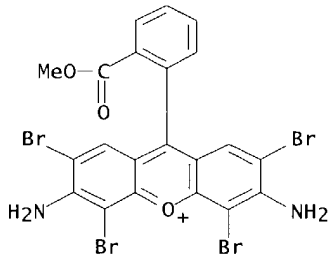
L29 ANSWER 18 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:453091 HCAPLUS
DOCUMENT NUMBER: 122:285634
TITLE: Selective photodynamic inactivation of a multidrug transporter by a cationic photosensitizing agent
AUTHOR(S): Kessel, D; Woodburn, K
CORPORATE SOURCE: School of Medicine, Wayne State University, Detroit, MI, 48201, USA
SOURCE: British Journal of Cancer (1995), 71(2), 306-10
CODEN: BJCAAI; ISSN: 0007-0920
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have characterized sites of photodamage catalyzed by the cationic photosensitizer tetrabromorhodamine 123, using P388 murine leukemia cells and a subline (P388/ADR) which has a multidrug resistance phenotype and hyperexpresses mdr1 mRNA for P-glycoprotein. Fluorescence emission spectra were consistent with sensitizer localization in hydrophobic regions of the P388 cell, and in more aq. loci in P388/ADR. Subsequent irradn. resulted in photodamage to the P388 cells, resulting in loss of viability. In contrast, P388/ADR cells were unaffected except for an irreversible inhibition of P-glycoprotein, leading to enhanced accumulation of daunorubicin and rhodamine 123 and a corresponding increase in daunorubicin cytotoxicity. These results are consistent with the premise that substrates for P-glycoprotein are confined to membrane loci assocd. with the transporter, and indicate a very limited migration of cytotoxic photoproducts in a cellular environment.
IT **83796-96-7**, Tetrabromo-rhodamine 123
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(photodynamic inactivation of multidrug transporter in leukemia cells by cationic photosensitizer tetrabromorhodamine 123 with visible light)
RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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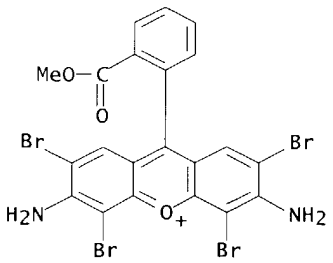
L29 ANSWER 19 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:18589 HCAPLUS
DOCUMENT NUMBER: 118:18589
TITLE: Mapping radiant energy distributions during laser irradiation of collagen phantoms by photolabeling with tetrabrominated rhodamine
AUTHOR(S): Jacques, Steven L.; Hasan, Tayyaba
CORPORATE SOURCE: Laser Biol. Res. Lab., Univ. Texas, Houston, TX, 77030, USA
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1992), 1646(Proc. Laser-Tissue Interact. III, 1992), 219-26
CODEN: PSISDG; ISSN: 0277-786X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A method is proposed for mapping laser light distributions in gel phantoms by measurement of the distribution of a fluorescent compd. that has been photolabeled to the gel by the laser irradiance. A preliminary study of photolabeling by an argon laser using tetrabrominated rhodamine (TBR) was conducted in collagen gel phantoms to illustrate the feasibility of the method. A discussion of the basic quant. relationships for anal. of measurements is presented.
IT **83796-96-7**
RL: BIOL (Biological study)
(photolabeling with, in laser radiation energy distribution mapping in collagen gel phantoms)
RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



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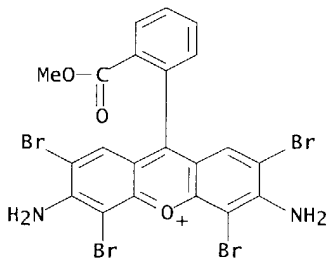
L29 ANSWER 20 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:146920 HCAPLUS
DOCUMENT NUMBER: 116:146920
TITLE: A test of the singlet oxygen mechanism of cationic dye photosensitization of mitochondrial damage
AUTHOR(S): Bunting, James R.
CORPORATE SOURCE: Baylor Res. Inst., Dallas, TX, 75226, USA
SOURCE: Photochemistry and Photobiology (1992), 55(1), 81-7
CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Arom. cationic dyes have a potential as photo-chemotherapeutic agents because they are selectively concd. into the mitochondria of cancerous cells. The mechanism of cytophototoxicity has been proposed to be primarily due to dye sensitized photogeneration of highly toxic singlet oxygen (1O2) at the mitochondria. This hypothesis was tested by measuring the relative phototoxicity of a collection of arom. cationic dyes towards respiring rat-liver mitochondria (RLM), upon addn. of 514 nm laser light. The effectiveness of dye photosensitization towards destruction of RLM function was assayed by its effect on the RLM membrane potential. Three phys. parameters of dye phototoxicity were independently measured and a relative phototoxicity calcd. assuming adherence of mechanism in the 1O2 hypothesis. Quantum yields of dye-sensitized 1O2 prodn. were estd., either from time-resolved luminescence measurements of photosensitized 1O2 formed, or by comparing rates of photobleaching of 1O2 trap; the relative partition of dye into mitochondrial lipid was detd. gravimetrically; and the optical d. of dye was detd. in a lipid like Triton X 100 micellar environment. Under the assumption of the 1O2 hypothesis, these parameters were used to predict a relative phototoxicity which was compared with that obsd. For 12 of the 14 dyes investigated, the obsd. and predicted phototoxicities were linearly correlated (r = 0.85), suggesting support of the 10- and 1000-fold more potent than preducted, suggesting an addnl. factor at play in their phototoxicity.

IT **83796-96-7**, Tetrabromo-rhodamine 123
RL: BIOL (Biological study)
(photosensitization by, of liver mitochondria, singlet oxygen mechanism of evaluation in)
RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

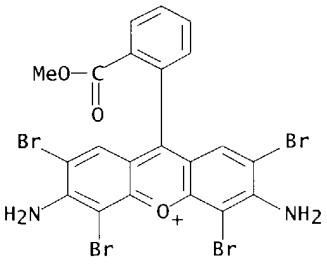
L29 ANSWER 21 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:473949 HCAPLUS
DOCUMENT NUMBER: 111:73949
TITLE: Rhodamine dyes as potential agents for photochemotherapy of cancer in human bladder carcinoma cells

AUTHOR(S): Shea, Christopher R.; Chen, Norah; Wimberly, Joanne; Hasan, Tayyaba
CORPORATE SOURCE: Dep. Dermatol., Harvard Med. Sch., Boston, MA, 02114, USA
SOURCE: Cancer Research (1989), 49(14), 3961-5
CODEN: CNREA8; ISSN: 0008-5472
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The phototoxicity in vitro of rhodamine 123 and tetrabromorhodamine 123 (TBR) was compared in order to assess the photochemotherapeutic potential of these compds. Exposure to 514.5-nm radiation from an Ar ion laser caused phototoxicity in MGH-U1 bladder carcinoma cells previously treated with either dye at 10 .mu.M for 30 min. As assessed by colony formation and cellular morphol., TBR was markedly more phototoxic than rhodamine 123, reflecting increased intersystem crossing of TBR to the triplet manifold via spin-orbital coupling induced by the heavy Br atoms. Photoreactions of TBR very efficiently generated singlet O (1O2) in soln.; furthermore, irradn. of TBR-treated cells was significantly more toxic when performed in the presence of deuterium oxide, an enhancer of damage caused by 1O2. Retention of fluorescence in TBR-treated cells was enhanced by irradn., indicating that a stable photoproduct may be formed in reaction with cellular components.

IT **83796-96-7**
RL: PRP (Properties)
(phototoxicity of, photochemotherapy of human bladder carcinoma in relation to)

RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L29 ANSWER 22 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:208583 HCAPLUS
DOCUMENT NUMBER: 110:208583
TITLE: Phototoxicity of rhodamine dyes
AUTHOR(S): Shea, Christopher R.; Chen, Norah; Hasan, Tayyaba
CORPORATE SOURCE: Massachusetts Gen. Hosp., Harvard Med. Sch., Boston, MA, 02114, USA
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1989), 997(Adv. Photochemother.), 48-57
CODEN: PSISDG; ISSN: 0277-786X
DOCUMENT TYPE: Journal
LANGUAGE: English

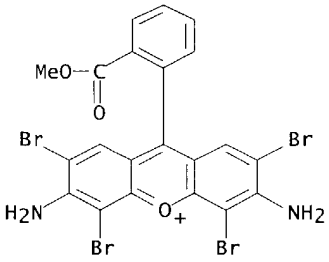
AB Rhodamine-123 (R123) and tetrabromo-R123 (TBR) have been evaluated in vitro as potential photosensitizers with laser radiation. R123 localizes selectively in mitochondria of MGH-U1 bladder carcinoma cells exposed to 10 .mu.M R123 for 30 min, and under these conditions R123 is a weak photosensitizer. Incubation with R123 for longer times enhances its

phototoxicity, and is assocd. with a modification of its intracellular localization. TBR is .apprx.100-fold more phototoxic than R123, as assessed either by [3H]thymidine uptake or vital staining. Actively proliferating cells are more sensitive to either R123 or TBR phototoxicity than are plateau-phase, confluent cultures.

IT **83796-96-7**
RL: PRP (Properties)
(phototoxicity of, to bladder carcinoma cells with laser radiation)

RN 83796-96-7 HCAPLUS

CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



● Cl-

L29 ANSWER 23 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1983:211699 HCAPLUS

DOCUMENT NUMBER: 98:211699

TITLE: Triplet anisotropy decay measurements of DNA internal motion

AUTHOR(S): Hogan, Michael; Wang, Johnny; Austin, R. H.

CORPORATE SOURCE: Dep. Biochem. Sci., Princeton Univ., Princeton, NJ, 08540, USA

SOURCE: Ciba Foundation Symposium (1983), 93(Mobility Funct. Proteins Nucleic Acids), 226-45
CODEN: CIBSB4; ISSN: 0300-5208

DOCUMENT TYPE: Journal

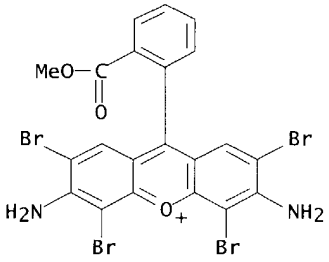
LANGUAGE: English

AB Triplet anisotropy decay techniques were used to measure the internal flexibility and overall rotational motions of DNA over a time range of 15 ns to 200 .mu.s. Nearly monodisperse DNA fragments with lengths varying from 65-600 base pairs were studied with the intercalating dye methylene blue as a triplet probe. The slow end-over-end tumbling of short DNA fragments (<165 base pairs) is as predicted for a rigid rod. A longer DNA fragment (600 base pairs) experiences slow segmental motions of its helix axis. At the earliest times, anisotropy decays more rapidly than expected for a rigid rod, suggesting that, when it is bound, methylene blue monitors fast internal motions of the helix. Since the rodlike end-over-end tumbling rules out fast bending motions (for short DNA fragments), the fast components of DNA anisotropy decay must be due to twisting motions of the helix, occurring with a time const. of .apprx.50 ns. The same techniques were used to measure the conformational flexibility of DNA in the nucleosome. It is concluded that, when the DNA helix is wrapped to form a nucleosome, it experiences substantial internal flexibility, occurring with a time const. of .apprx.30 ns. The amplitude and time-scale of this motion are similar to that seen in the uncomplexed DNA helix.

IT **83796-96-7**
RL: BIOL (Biological study)
(triplet anisotropy decay of, in DNA, internal motions in relation to)

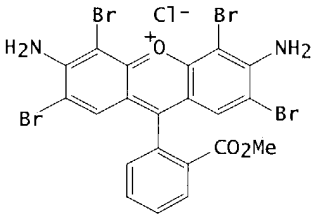
RN 83796-96-7 HCAPLUS

CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

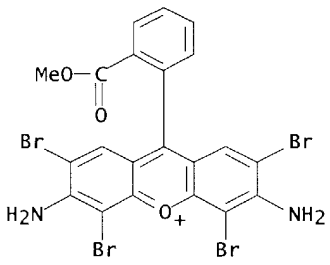
L29 ANSWER 24 OF 24 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:1816 HCAPLUS
DOCUMENT NUMBER: 98:1816
TITLE: DNA motions in the nucleosome core particle
AUTHOR(S): Wang, J.; Hogan, M.; Austin, R. H.
CORPORATE SOURCE: Dep. Biochem. Sci., Princeton Univ., Princeton, NJ, 08544, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1982), 79(19), 5896-900
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Time-resolved triplet-state anisotropy decay techniques employing the intercalating agents, methylene blue and tetrabromorhodamine 123 chloride (I), the latter prepd. by bromination of rhodamine 123, were used to measure the conformational flexibility of DNA in the chicken erythrocyte nucleosome. In a nucleosome, the DNA helix experiences substantial internal flexibility, which occurs with a time const. of .apprx.30 ns. The data can be fit well by a modified version of the Barkley-Zimm model for DNA motion, allowing only DNA twisting motions and the overall tumbling of the nucleosome. That fit yields a calcd. torsional rigidity equal to 1.8 .times. 10-19 erg-cm, a value equal to that measured for uncomplexed DNA. Such similarity suggests that large, fast twisting motions of the DNA helix persist, nearly unaltered, when DNA is wrapped to form a nucleosome.
IT **83796-96-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as DNA intercalating agent)
RN 83796-96-7 HCAPLUS
CN Xanthylium, 3,6-diamino-2,4,5,7-tetrabromo-9-[2-(methoxycarbonyl)phenyl]-,

chloride (9CI) (CA INDEX NAME)



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                 OR 81-88-9/BI)
L62           2 SEA FILE=REGISTRY ABB=ON  PLU=ON  "4,5-DIBROMO" AND "BIS(DIETHY
                LAMINO)"
L63           5 SEA FILE=REGISTRY ABB=ON  PLU=ON  L39 AND BR=2
L64           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L62
L65           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L63
L66           3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L64 OR L65)


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L66  ANSWER 1 OF 3  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2002:777919  HCAPLUS
DOCUMENT NUMBER:          137:280622
TITLE:                    Halogenated rhodamine dye derivatives and their
                          therapeutic applications
INVENTOR(S):              Habi, Abdelkrim; Gravel, Denis; Villeneuve, Luc;
                          Forte, Jean-Pierre; Su, Hongsheng; Vaillancourt, Marc
PATENT ASSIGNEE(S):       Theratechnologies Inc., Can.
SOURCE:                   PCT Int. Appl., 117 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     WO 2002079183      A1   20021010       WO 2002-CA438    20020327
     WO 2002079183      C1   20030220
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1276734         A1   20030122       EP 2002-708105   20020327
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002004489      A    20030401       BR 2002-4489     20020327
     US 2003212126      A1   20031113       US 2003-297088   20030530
PRIORITY APPLN. INFO.:                    CA 2001-2342675  A  20010402
                                          US 2001-822223   A  20010402
                                          WO 2002-CA438    W  20020327
OTHER SOURCE(S):          MARPAT 137:280622
AB   Bromo derivs. of rhodamine 110, rhodamine B, and rhodamine 6G and other
     halo rhodamine derivs. are useful as intermediates and as bactericides and
     antiviral agents and in the treatment of immunol. disorders.  In an
     example, rhodamine B Me ester was dihydrogenated and then brominated and
     oxidized and treated with acetic acid to provide the purple acetate salt
     of 2,7-dibromorhodamine B Me ester.
IT   177989-33-2
     RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (bacteriostatic agent; halogenated rhodamine dye derivs. and their
        therapeutic applications)
RN   177989-33-2  HCAPLUS
CN   Benzoic acid, 2-(3,6-diamino-4,5-dibromo-9H-xanthen-9-yl)-, methyl ester
     (9CI)  (CA INDEX NAME)
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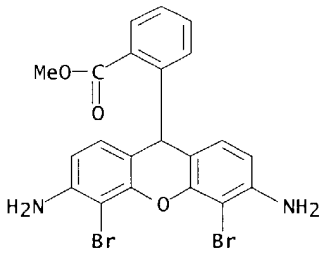
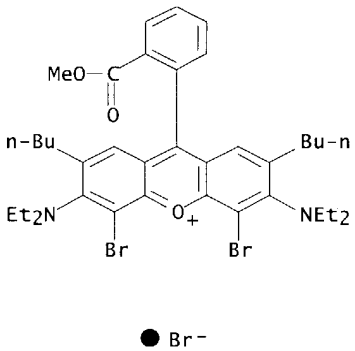


IT **467232-23-1P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(red dye; prodn. of halogenated rhodamine dye derivs. and their therapeutic applications)
RN 467232-23-1 HCAPLUS
CN Xanthylium, 4,5-dibromo-2,7-dibutyl-3,6-bis(diethylamino)-9-[2-(methoxycarbonyl)phenyl]-, bromide (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L66 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:265273 HCAPLUS
DOCUMENT NUMBER: 134:292146
TITLE: Rhodamine derivatives for photodynamic diagnosis and treatment
INVENTOR(S): Roy, Denis-Claude; Guimond, Martin; Molfino, Nestor A.
PATENT ASSIGNEE(S): Universite de Montreal, Can.; Hopital Maisonneuve-Rosemont
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001024824	A1	20010412	WO 2000-CA1142	20001003

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,

SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

BR 2000014135	A	20020521	BR 2000-14135	20001003
EP 1267931	A1	20030102	EP 2000-965683	20001003
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003510372	T2	20030318	JP 2001-527823	20001003

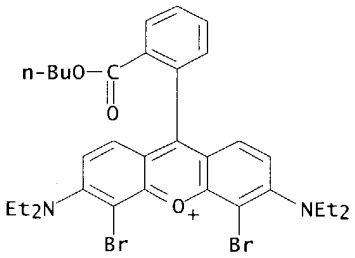
PRIORITY APPLN. INFO.: US 1999-157790P P 19991005
WO 2000-CA1142 W 20001003

AB The present invention relates to the use of the photoactivable derivs. for the photodynamic treatment for the selective destruction and/or inactivation of immunol. reactive cells without affecting the normal cells and without causing systemic toxicity for the patient, wherein appropriate intracellular levels of said derivs. are achieved and irradn. of a suitable wavelength and intensity is applied. Examples are given of the selective phototoxicity of rhodamine derivs. against K562 cells, CEM cells, PHA-activated lymphocytes, activated CD4+ and CD8+ cells and human B cells. Immunol. disorders, including graft-vs-host disease are treated with photodynamic therapy.

IT **333957-96-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(rhodamine derivs. for photodynamic diagnosis and treatment of immunol. disorders)

RN 333957-96-3 HCAPLUS

CN Xanthylium, 4,5-dibromo-9-[2-(butoxycarbonyl)phenyl]-3,6-bis(diethylamino)-, chloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L66 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1996:379805 HCAPLUS
DOCUMENT NUMBER:	125:52522
TITLE:	Novel rhodamine derivatives for photodynamic therapy of cancer and in vitro purging of the leukemias
INVENTOR(S):	Gaboury, Louis; Giasson, Richard; Li, Tiechao; Gupta, Ajay Kumar; Villeneuve, Luc
PATENT ASSIGNEE(S):	Universite De Montreal, Can.
SOURCE:	PCT Int. Appl., 37 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9607431	A1	19960314	WO 1995-CA485	19950816
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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CA 2197435	AA	19960314	CA 1995-2197435	19950816
AU 9532488	A1	19960327	AU 1995-32488	19950816
AU 688100	B2	19980305		
EP 773794	A1	19970521	EP 1995-928907	19950816
EP 773794	B1	20010620		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
BR 9508779	A	19971223	BR 1995-8779	19950816
JP 10505349	T2	19980526	JP 1995-509057	19950816
AT 202286	E	20010715	AT 1995-928907	19950816
ES 2160173	T3	20011101	ES 1995-928907	19950816
PT 773794	T	20011228	PT 1995-95928907	19950816
US 5773460	A	19980630	US 1996-674247	19960701
GR 3036636	T3	20011231	GR 2001-401494	20010917

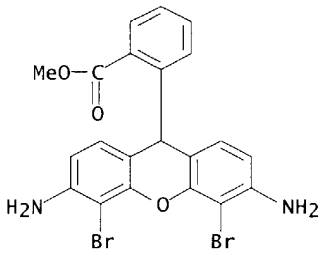
PRIORITY APPLN. INFO.: US 1994-300179 A 19940902
WO 1995-CA485 W 19950816

AB The present invention relates to novel photoactivable rhodamine derivs. for enhancing high quantum-yield prodn. and singlet oxygen generation upon irradn. with light while maintaining desirable differential retention of rhodamine between normal and cancer cells, said derivs. are selected from the group consisting of 4,5-dibromorhodamine 123 (2-(4,5-dibromo-6-amino-3-imino-3H-xanthen-9-yl)-benzoic acid Me ester hydrochloride); 4,5-dibromorhodamine 123 (2-(4,5-dibromo-6-amino-3-imino-3H-xanthen-9-yl)-benzoic acid Et ester hydrochloride); 4,5-dibromorhodamine 123 (2-(4,5-dibromo-6-amino-3-imino-3H-xanthen-9-yl)-benzoic acid octyl ester hydrochloride); 4,5-dibromorhodamine 110 Bu ester (2-(4,5-dibromo-6-amino-3-imino-3H-xanthen-9-yl)-benzoic acid Bu ester hydrochloride); rhodamine B Bu ester (2-(6-Et amino-3-Et imino-3H-xanthen-9-yl)-benzoic acid Bu ester hydrochloride); and photoactivable derivs. thereof; whereby photoactivation of the derivs. induces cell killing while unactivated derivs. are substantially non-toxic to cells. Also, the present invention relates to the use of the photoactivable derivs. of the present invention for the photodynamic therapy of a cancer patient by destroying human cancer cells, wherein appropriate intracellular levels of the derivs. are achieved and irradn. with light of a suitable wavelength is applied. The present invention also relates to a method for the photodynamic therapy of a patient suffering from leukemias, disseminated multiple myelomas or lymphomas.

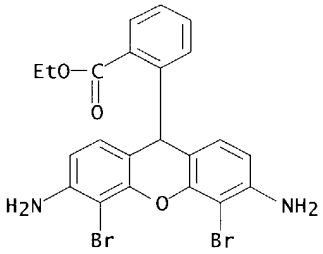
IT **177989-33-2 177989-34-3 177989-35-4**
177989-36-5 177989-37-6
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(rhodamine derivs. for photodynamic therapy of cancer and leukemias)

RN 177989-33-2 HCAPLUS

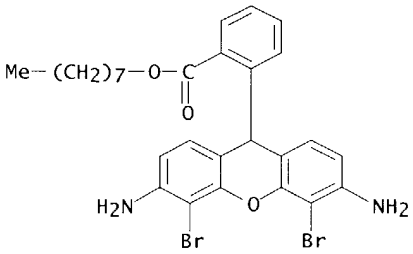
CN Benzoic acid, 2-(3,6-diamino-4,5-dibromo-9H-xanthen-9-yl)-, methyl ester (9CI) (CA INDEX NAME)



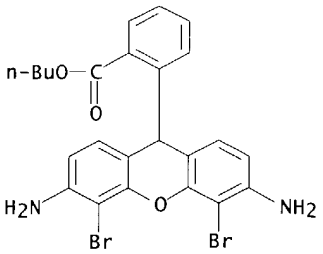
RN 177989-34-3 HCAPLUS
CN Benzoic acid, 2-(3,6-diamino-4,5-dibromo-9H-xanthen-9-yl)-, ethyl ester (9CI) (CA INDEX NAME)



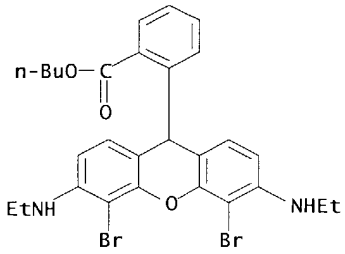
RN 177989-35-4 HCAPLUS
CN Benzoic acid, 2-(3,6-diamino-4,5-dibromo-9H-xanthen-9-yl)-, octyl ester (9CI) (CA INDEX NAME)



RN 177989-36-5 HCAPLUS
CN Benzoic acid, 2-(3,6-diamino-4,5-dibromo-9H-xanthen-9-yl)-, butyl ester (9CI) (CA INDEX NAME)



RN 177989-37-6 HCAPLUS
CN Benzoic acid, 2-[4,5-dibromo-3,6-bis(ethylamino)-9H-xanthen-9-yl]-, butyl ester (9CI) (CA INDEX NAME)



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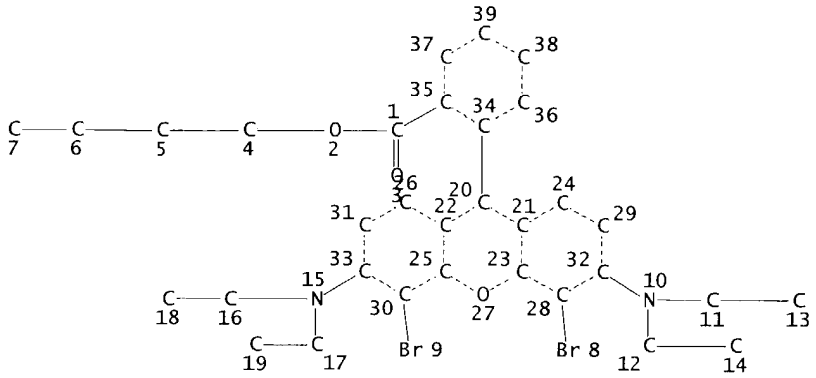
L75 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE
L77 1 SEA FILE=REGISTRY FAM FUL L75

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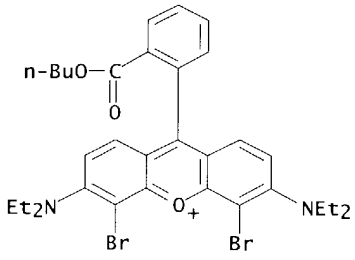
L77 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Xanthylium, 4,5-dibromo-9-[2-(butoxycarbonyl)phenyl]-3,6-bis(diethylamino)-, chloride (9CI)
MF C32 H37 Br2 N2 O3 . Cl



ALL ANSWERS HAVE BEEN SCANNED